2-Pentanethiol, 2-methyl-

Other names: 2-Methyl-2-pentanethiol
2-methylpentane-2-thiol
Inchi: InChI=1S/C6H14S/c1-4-5-6(2,3)7/h7H,4-5H2,1-3H3
InchiKey: ISUXQQTXICTKOV-UHFFFAOYSA-N
Formula: C6H14S
SMILES: CCCC(C)(C)S
Mol. weight [g/mol]: 118.24
CAS: 1633-97-2

Physical Properties

Property code	Value	Unit	Source
chl	-4775.62 ± 0.84	kJ/mol	NIST Webbook
gf	31.87	kJ/mol	Joback Method
hf	-148.00 ± 1.00	kJ/mol	NIST Webbook
hfl	-187.90 ± 0.96	kJ/mol	NIST Webbook
hfus	7.92	kJ/mol	Joback Method
hvap	39.90	kJ/mol	NIST Webbook
hvap	40.00 ± 0.10	kJ/mol	NIST Webbook
hvap	40.00 ± 0.20	kJ/mol	NIST Webbook
log10ws	-2.52		Crippen Method
logp	2.495		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
rinpol	930.00		NIST Webbook
tb	396.31	K	Joback Method
tc	598.05	K	Joback Method
tf	196.26	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.50	J/mol×K	396.31	Joback Method
cpg	219.51	J/mol×K	429.93	Joback Method

cpg	231.80	J/mol×K	463.56	Joback Method
cpg	243.40	J/mol×K	497.18	Joback Method
cpg	254.34	J/mol×K	530.80	Joback Method
cpg	264.66	J/mol×K	564.43	Joback Method
cpg	274.38	J/mol×K	598.05	Joback Method
hvapt	38.00	kJ/mol	383.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49054e+01
Coeff. B	-3.76948e+03
Coeff. C	-5.75790e+01
Temperature range (K), min.	315.45
Temperature range (K), max.	450.48

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1633972&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume